A study of Numerical Dispersion for Helmholtz equation in one dimension by Z transform

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Overview

Plan

Numerical Dispersion

Helmholtz equation gives the long-time behavior of the wave equation

$$(\partial_t^2 - c^2\Delta)\,\mathbf{U}(t,x) \;=\; \mathbf{f}(x)\,e^{-i\omega t}$$

where $c =$ speed of propagation
$\frac{\omega}{2\pi} =$ time freq. of the excitation

Look for time-harmonic sol with the same freq

$$\mathbf{U}(t,x) = \mathbf{u}(x)\,e^{-i\,\omega\,t}$$

thus $\mathbf{u}$ solves the Helmholtz

$$(-\Delta - \tfrac{\omega^2}{c^2})\,\mathbf{u} = \mathbf{f}$$

$\kappa := \frac{\omega}{c}$ the wave number .

Fund. sols of $(-\Delta - \kappa^2)\,\mathbf{u} = 0$ are

$$e^{i\,\kappa\,x} \quad , \quad e^{-i\,\kappa\,x} \quad .$$

corresponding to harmonic plane wave

$e^{i(\,\kappa\,x-\omega t)}$ propagating from L to R
$e^{-i(\,\kappa\,x-\omega t)}$ propagating from R to L

with phase velocity $\frac{\omega}{\kappa} =$ constant speed c

depending only on material properties

and not ω

No dispersion behavior

for the exact solution.

The numerical solution associated Finite Element or Finite Difference

$$u_h = e^{-i(\kappa_h x - \omega t)}$$

with numerical wavenumber

$$\kappa_h = \kappa_h(\kappa h) = \kappa_h(\tfrac{\omega}{c} h) \neq \tfrac{\omega}{c},$$

depending on ω.

The numerical phase velocity

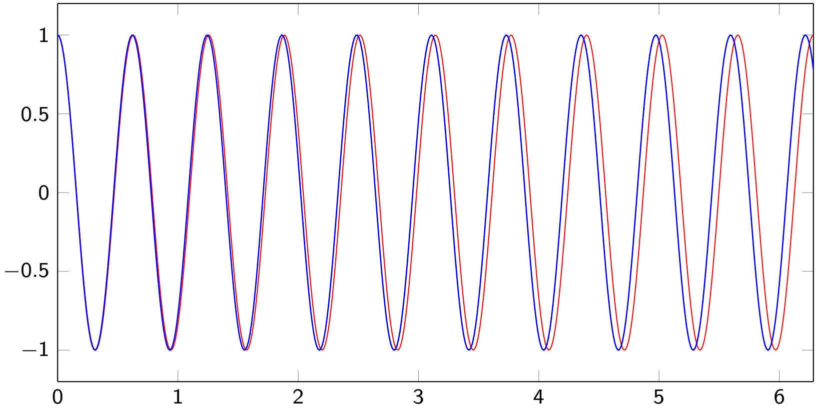
$$\frac{\omega}{\kappa_h} \neq \text{constant speed } c$$

and depends on ω

Dispersive behavior of

the numerical solution

Numerical Dispersion for Finite Difference Order 2

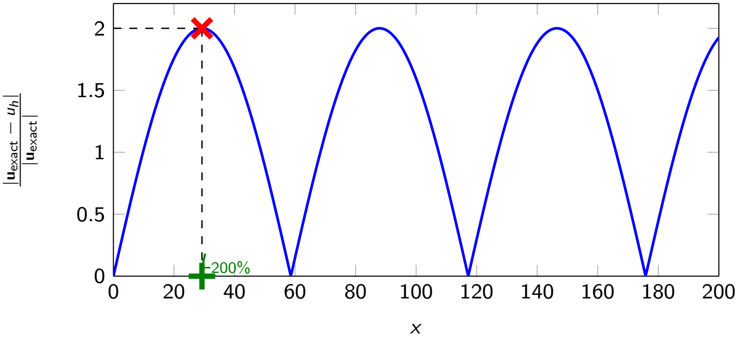


$\mathrm{Re}\ \mathbf{u}_{\text{exact}} = \cos(\kappa x)$; $\mathrm{Re}\ u_h = \cos(\kappa_h x)$

$$\kappa = 10\ ,\ h = 0.05\ ,\ \kappa_h = \frac{2}{h}\arcsin\left(\frac{\kappa h}{2}\right) \sim 10.10721\ .$$

Exact phase velocity $= c$; Numerical phase velocity $= \dfrac{\omega}{\kappa_h} = c\,\dfrac{\kappa}{\kappa_h} = c\,\dfrac{\frac{\kappa h}{2}}{\arcsin\left(\frac{\kappa h}{2}\right)} \sim 0.98939\, c$

Numerical Dispersion for Finite Difference Order 2



Relative error between $\mathbf{u}_{\text{exact}} = e^{i\,\kappa\,x}$ and $u_h = e^{i\,\kappa_h\,x}$

The first maximum is reached in red (❌) and corresponds to 200% error.

Methodology and Results

Goal

Study the phase difference between

the analytic wavenumber κ and

the numerical one κ_h associated with the discretization of the variational problem by Continuous Galerkin FEM for any order.

⋆ Discretization is on $\mathbb{R}$,
$\Rightarrow$ the pollution is studied in *isolation with the effect of spurious reflection at the boundary* .

⋆ Use blocking + Z-transform to transform system of two-sided infinite recurrence relations into one matrix-vector equation

$$\mathcal{A}(\kappa^2 h^2, z)\, W(\kappa, z) \;=\; h\, z\, H(z).$$

⋆ Identity the numerical wavenumber κ_h with the angle of the (analytic) poles of

$$[\mathcal{A}(\kappa^2 h^2, z)]^{-1}$$

⋆ For any order r, obtain dispersion analysis in the form of an analytic expansion,

$$\kappa_h\, h \;=\; \kappa\, h \;+\; \kappa\, h\, \mathrm{O}\Big((\kappa\, h)^{2r}\Big).$$

$$\underset{\text{in } \kappa h}{\text{analytic}} \quad \frac{\kappa_h - \kappa}{\kappa} \;\leq\; C(r)\, (\kappa\, h)^{2r}.$$

⋆ Use Guillaume's algorithm to numerically calculate the poles, and hence κ_h.

Toy Example : Numerical Dispersion analysis for FD order 2

Uniform discretization of $\mathbb{R}$ with step size h by nodes

$$x_n = n\,h \quad , \quad n \in \mathbb{Z} \quad .$$

Recurrence relation given by second order Finite Difference

$$-u_{n-1} + (2 - \kappa^2 h^2)\, u_n - u_{n+1} = 0 \quad , \quad n \in \mathbb{Z}.$$

(Analytic) wavenumber κ controls the oscillatory behavior of u_{exact},

$$\mathbf{u}_{\text{exact}}(x) \;=\; a_+\, e^{i\,\kappa\,x} \;+\; a_-\, e^{-i\,\kappa\,x} \quad .$$

The **characteristic polynomial** of the recurr. relation,
$$z^2 - (2 - \kappa^2 h^2)\, z + 1 = 0 \quad ,$$

for $0 \le \kappa h < 2$, has conjugate complex roots of norm 1:

$$e^{i\,\gamma_h} \quad , \quad e^{-i\,\gamma_h} \quad .$$

The numerical wave number

$$\kappa_h := \frac{\gamma_h}{h}$$

controls the oscillatory behavior of numerical solution,

$$\begin{aligned} u_n \;&=\; a_+ e^{i\,\frac{\gamma_h}{h}\,(nh)} \;+\; a_- e^{-i\,\frac{\gamma_h}{h}\,(nh)} \\ &=\; a_+\, e^{i\,\kappa_h\,x} \;+\; a_-\, e^{-i\,\kappa_h\,x} \quad , \\ x &= n\,h \quad . \end{aligned}$$

Solution of the recurrence relation :

$$u_n \;=\; a_+\, e^{i\,\gamma_h\,n} \;+\; a_-\, e^{-i\,\gamma_h\,n} \quad .$$

A toy example (cnt)

$e^{i\gamma_h}$ solves $z^2 - (2-\kappa^2 h^2)z + 1 = 0$

$$\Rightarrow e^{i\gamma_h} \text{ satifies } z-(2-\kappa^2 h^2)+z^{-1} = 0$$

$$\Rightarrow \quad \underbrace{e^{i\gamma_h} + e^{-i\gamma_h}}_{2\cos(\gamma_h)} = 2-\kappa^2 h^2$$

$$\Rightarrow \quad 2\left(1-\cos(\gamma_h)\right) = \kappa^2 h^2$$

$$\Rightarrow \quad 4\sin^2(\tfrac{1}{2}\gamma_h) = \kappa^2 h^2$$

$\kappa > 0$ and h is chosen small enough so that $\sin(\frac{1}{2}\gamma_h) > 0$.

$$\sin(\tfrac{1}{2}\gamma_h) = \tfrac{1}{2}\kappa\, h$$

$$\Rightarrow \quad \gamma_h = 2\arcsin(\tfrac{1}{2}\kappa\, h)$$

$$\kappa_h = \frac{2}{h}\arcsin\left(\frac{1}{2}\kappa\, h\right) \quad .$$

For $|\kappa h| < 2$,

$$\kappa_h = \frac{2}{h}\arcsin\left(\frac{1}{2}\kappa\, h\right)$$

$$= \frac{2}{h}\sum_{n=0}^{\infty}\frac{(2n)!}{4^n(n!)^2(2n+1)}\frac{1}{2\cdot 4^n}(\kappa\, h)^{2n+1}$$

Dispersion analysis

$$\delta_h = \kappa_h - \kappa$$

$$= \frac{1}{24}\kappa^3 h^2 + \mathcal{E}_h(\kappa\, h) \quad , \quad |\kappa\, h| < 2.$$

$\mathcal{E}_h$ is analytic ,

$$\mathcal{E}_h(\kappa\, h) = \kappa\, h \sum_{n=2}^{\infty}\frac{(2n)!}{4^{2n}(n!)^2(2n+1)}(\kappa\, h)^{2n}$$

$$= \kappa\, h\ \mathrm{O}\left((\kappa\, h)^4\right) \quad ; \quad |\kappa\, h| < 2 \quad .$$

Results from literature

Theoretical proof that gives an upper bound of the phase difference :

Theorem (Ihlenburg-Babushka)

For $r \geq 1$, if $\dfrac{h\,\kappa}{r} < 1$, for the CG FEM discretization of the BVP

$$\begin{cases} -u'' - \kappa^2\, u = f \;, \quad on \;\; (0,1) \\ \\ u(0) = 0 \quad ; \quad u'(1) - i\kappa\, u(1) = 0 \end{cases}$$

the difference between the continous wave number κ and the numerical one κ_h is bounded above by,

$$\left|\kappa_h - \kappa\right| \quad \leq \quad \kappa\, C \left(\frac{e}{4}\right)^{2r} \frac{(\pi r)^{-1/2}}{4} \left(\frac{\kappa h}{2r}\right)^{2r} \quad .$$

Here, C is a constant not depending on κ, h and r.

Other References :
By numerical results : Thompson-Pinsky , Harari-Hughes ...

Plan

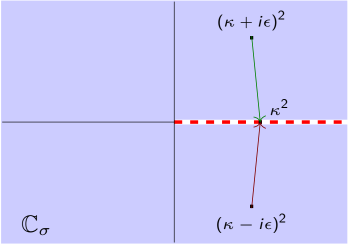
Functional Analysis view point

Δ is an unbounded op. on $L^2(\mathbb{R})$ with domain $H^2(\mathbb{R})$

$\boldsymbol{\sigma}(-\Delta) = \boldsymbol{\sigma}_{\text{continuous}}(-\Delta) = \mathbb{R}^+$: *purely continuous.*

Inverse of $-\Delta - \sigma$ is a resolvent $\mathcal{R}(\sigma)$ of Δ.

$$(-\Delta - \sigma)^{-1} : L^2(\mathbb{R}) \to L^2(\mathbb{R}) \text{ bounded}, \ \sigma \in \mathbb{C} \setminus \mathbb{R}^+$$



Highlighted reg. $\mathbb{C} \setminus \mathbb{R}^+$ = resolv. set of $-\Delta$

No eigenvalue (no eigenfunction in $L^2(\mathbb{R})$) .

$$(-\Delta - \sigma)u = 0 \text{ in } L^2(\mathbb{R}) \quad \Rightarrow \quad (|\xi|^2 - \sigma)\widehat{u} = 0$$

$$\Rightarrow \quad \widehat{u} = 0 \quad \Rightarrow \quad u = 0 \text{ in } L^2(\mathbb{R}).$$

There are 'generalized ' eigenfunctions $\in \mathcal{S}'(\mathbb{R})$

$$(-\Delta - \sigma)u = 0 \text{ in } \mathcal{S}'(\mathbb{R}) \quad \Rightarrow \quad (|\xi|^2 - \sigma)\widehat{u} = 0$$

$$\Rightarrow \widehat{u} = a_- \delta_{-\sqrt{\sigma}} + a_+ \delta_{\sqrt{\sigma}} \quad \Rightarrow u = \underbrace{a_- e^{-i\sqrt{\sigma}x} + a_+ e^{i\sqrt{\sigma}x}}_{\notin L^2(\mathbb{R})}.$$

$$\boxed{\sigma \notin \mathbb{R}^+}$$

The variational form is coerc. in $L^2(\mathbb{R})$

Get $\exists!$ of sol in $L^2(\mathbb{R})$ by Fourier transf.

$$(-\Delta - \sigma)u = f \text{ in } L^2(\mathbb{R})$$

$$\Rightarrow u = \mathcal{F}^{-1} \frac{1}{|\xi|^2 - \sigma} \mathcal{F} f$$

$$\Rightarrow \quad \sigma(\Delta) \subset \mathbb{R}^+.$$

$$\boxed{\sigma = \kappa^2, \kappa \in \mathbb{R}^+}$$

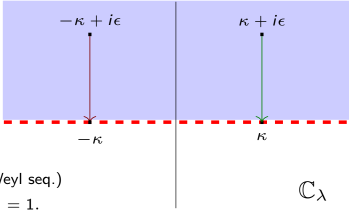
Construct a seq. w_n of 'almost eigenf.' (Weyl seq.)

$$\|(-\Delta - \lambda)w_n\|_{L^2(\mathbb{R})} \to 0 \,; \ \|w_n\|_{L^2(\mathbb{R})} = 1.$$

This prevents the existence of bounded

$$(-\Delta - \sigma)^{-1} \text{ in } L^2(\mathbb{R}) \text{ for } \sigma \in [0, +\infty).$$

$$\Rightarrow \ \mathbb{R}^+ \subset \sigma(-\Delta).$$



Complex plane $\lambda = \sqrt{\sigma}$

Limiting absorption principle

Explicit formula

By separation of variables, obtain

$$G_\epsilon(x) = \frac{e^{i\sqrt{\kappa^2+i\epsilon}\,|x|}}{2\,i\,\sqrt{\kappa^2+i\epsilon}}$$ as the fund. sol. to

$$(-\Delta - (\kappa^2 + i\epsilon))\, G_\epsilon = \delta(y)\ ,\ \kappa, \epsilon \in \mathbb{R}^+.$$

The unique solution in $L^2(\mathbb{R})$ is given by

$$\mathbf{u}_\epsilon = \int_{-\infty}^{\infty} G_\epsilon(x-y)\ f(y)\, dy;$$

For each x ,

$$G_\epsilon(x) \xrightarrow[\epsilon\to 0]{\text{point wise}} G_{\text{outgoing}}(x) := \frac{e^{i\,\kappa\,|x|}}{2\,i\,\kappa}.$$

$$\mathbf{u}_\epsilon \xrightarrow[\epsilon\to 0]{} \mathbf{u}_{\text{outgoing}} := G_{\text{outgoing}} \star \mathbf{f} \text{ in } H^2_{\text{loc}}(\mathbb{R}).$$

gives **the outgoing solution** to

$$(-\Delta - \kappa^2)\mathbf{u} = \mathbf{f}\ ,\ \mathbf{f} \in L^2_c(\mathbb{R}).$$

The Sommerfeld radiation condition : The outgoing solution satisfies

$$\begin{cases} \lim_{x\to\infty} |\frac{1}{i} u'(x) - k u(x)| = 0 \\ \lim_{x\to-\infty} |\frac{1}{i} u'(x) + k u(x)| = 0 \end{cases}.$$

Analytic Continuation

For $\mathbf{f} \in \mathcal{C}_c^\infty(\mathbb{R})$, $\widehat{\mathbf{f}}$ has an analytic extension to $\mathbb{C}$.

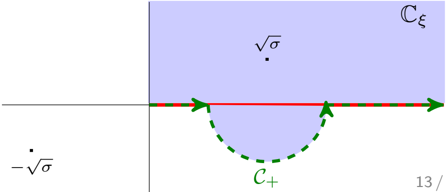
For $\sigma \in \mathbb{C}$ with $\operatorname{Re}\sigma > 0\ ,\ \operatorname{Im}\sigma > 0$, the unique sol. in $L^2(\mathbb{R})$ to $(-\Delta - \sigma)\mathbf{u} = \mathbf{f}$ is

$$\mathbf{u}(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{ix\cdot\xi}\,\frac{\widehat{\mathbf{f}}(\xi)}{|\xi|^2 - \sigma}\, d\xi = \frac{1}{2\pi}\left(\int_{-\infty}^{0} + \int_0^\infty\right)\ldots$$

$$= \frac{1}{2\pi}\int_0^\infty \left[e^{ix\cdot\xi}\widehat{\mathbf{f}}(\xi) + e^{-ix\cdot\xi}\widehat{\mathbf{f}}(-\xi)\right]\frac{1}{|\xi|^2 - \sigma}\, d\xi$$

Deform $[0,\infty)$ to $\mathcal{C}_+$, and get analytic continuation to $\{\sigma : \operatorname{Re}\sigma > 0\}$

$$\mathbf{u}_{\text{outgoing}}(x) = \frac{1}{2\pi}\int_{\mathcal{C}_+} \frac{e^{ix\cdot\xi}\widehat{\mathbf{f}}(\xi) + e^{-ix\cdot\xi}\widehat{\mathbf{f}}(-\xi)}{\xi^2 - \sigma}\, d\xi$$



Plan

3. Discretization of the problem on $\mathbb{R}$

Discretization

The real line $\mathbb{R}$ is partitioned into intervals of length h

$$I_J = [y_J, y_{J+1}]\,,\ J \in \mathbb{Z}.$$

the geometrical nodes

$$y_J := J\,h$$

For a method of order r, the intervals are further partitioned by global interpolation nodes

$$x_{J,k} := (J + \tfrac{k}{r})h$$

$$J \in \mathbb{Z}\,,\ 0 \le k < r.$$

Discrete solution :

$$u_h = \sum_{J\in\mathbb{Z},0\le k<r} u_{J,k}\,\phi_{J,k}\,.$$

A global basis for

$$\mathbb{P}_r = \{p \in C^0(\mathbb{R}) \mid p|_{I_J} \in P_r(I_J)\,,\ \forall J \in \mathbb{Z}\}$$

is given by $\phi_{J,k}$-s defined on $\mathbb{R}$ by

$$k = 0:\ \phi_{J,0}(x) := \begin{cases} \hat\phi_0(F_J^{-1}x) & ,\ x \in I_J \\ \hat\phi_r(F_{J-1}^{-1}x) & ,\ x \in I_{J-1} \\ 0 & ,\ \text{otherwise} \end{cases}\ ;$$

$$0 < k < r:\ \phi_{J,k}(x) := \begin{cases} \hat\phi_k(F_J^{-1}x) & ,\ x \in I_J \\ 0 & ,\ \text{otherwise} \end{cases}.$$

Ref Lagragian poly of deg r on [0,1] :

$$\hat\phi_i(\hat x) := \prod_{\substack{0\le j\le r\\ j\ne i}} \frac{(\hat x - \hat x_j)}{(\hat x_i - \hat x_j)}\quad.$$

Isomorphism between reference interval and I_J

$$F_J : [0,1] \to I_J\,,\ \hat x \mapsto hx + y_J\ ,\ \ J \in \mathbb{Z}.$$

Variational problem

Bilinear form for $v, w \in H^1(\mathbb{R})$,

$$a\,(v, w) := \int_{-\infty}^{\infty} v'(x)\, w'(x)\, dx - \kappa^2 \int_{-\infty}^{\infty} v(x)\, w(x)\, dx.$$

Discrete solution $u_h = \sum_{I\in\mathbb{Z}\,,\,0\le\ell<r} u_{I,\ell}\, \phi_{I,\ell}$ satisfies,

$$a\,(u_h\ ,\ \phi_{J,k}) \;=\; \int_{-\infty}^{\infty} \mathbf{f}(x)\, \phi_{J,k}(x)\, dx \quad , \quad \forall\, \phi_{J,k}\ , J \in \mathbb{Z}\ ,\ 0 \le k < r.$$

Local mass matrix $\widehat{M}$ of size $(r+1)\times(r+1)$

$$\widehat{M}_{ij} = \mathrm{a_M}(\hat{\phi}_i, \hat{\phi}_j) \quad , \quad 0 \le i,j \le r.$$

Local stiff matrix $\widehat{S}$ of size $(r+1)\times(r+1)$

$$\widehat{S}_{ij} = \mathrm{a_S}(\hat{\phi}_i, \hat{\phi}_j) \quad , \quad 0 \le i,j \le r.$$

$$\mathcal{M}_{ij}(w) := \widehat{S}_{ij} - w\widehat{M}_{ij} \quad , \quad 0 \le i,j \le r.$$

For $f, g \in H^1(0,1)$

$$\mathrm{a_S}(f,g) = \int_0^1 f'(\hat{x})\, g'(\hat{x})\, d\hat{x}$$

For $f, g \in L^2(0,1)$,

$$\mathrm{a_M}(f,g) = \int_0^1 f(\hat{x})\, g(\hat{x})\, d\hat{x}.$$

Recurrence relations

$$u_h = \sum_{J\in\mathbb{Z},0\le k<r} u_{J,k}\,\phi_{J,k} \qquad \begin{array}{r} a(u_h,\phi_{J,k}) = f_{J,k} \\ J\in\mathbb{Z} \quad , \quad 0\le k<r. \end{array} \tag{1}$$

The coefficients $u_{J,k}$-s satify the following system of r recurrence relations:

Those at levels Jr, $J\in\mathbb{Z}$ come from applying (1) to $\phi_{J,0}$ (at geo. nodes)

$$\sum_{\ell=0}^{r-1}\mathcal{M}_{r\ell}\,u_{J-1,\ell} + 2\mathcal{M}_{00}\,u_{J,0} + \sum_{\ell=1}^{r-1}\mathcal{M}_{0\ell}\,u_{J,\ell} + \mathcal{M}_{0r}\,u_{J+1,0} = h\,f_{J,0};$$

The remaining types at levels $Jr+k$, with $0<k<r$, are obtained from applying (1) to $\phi_{J,k}$ (at interpolation nodes)

$$\sum_{\ell=0}^{r-1}\mathcal{M}_{k\ell}\,u_{J,\ell} + \mathcal{M}_{kr}\,u_{J+1,0} = h\,f_{J,k} \quad ; \quad 0<k<r.$$

$$f_{J,k} := \int_{-\infty}^{\infty}\mathbf{f}(x)\,\phi_{J,k}(x); \quad J\in\mathbb{Z},\ 0\le k<r.$$

Plan

4. Summary of techniques and results

(Two-sided) Z-transforms for scalar sequence $u = \{u_n\}_{n\in\mathbb{Z}}$

	Version θ	**Version z**
Definition	$[Zu](\theta) := \sum_{n=-\infty}^{\infty} u_n\, e^{2\pi i n\theta}$ if the RHS converges	$[Zu](z) := \sum_{n=-\infty}^{\infty} u_n\, z^n$ if the RHS converges
$u \in l^2(\mathbb{Z})$	$[Zu](\theta)$ is periodic in θ $Z : l^2(\mathbb{Z}) \longrightarrow L^2(0,1)$ is an isometry	$Z : l^2(\mathbb{Z}) \longrightarrow L^2(\mathbb{S}^1)$ is an isometry
	u_n is the n-th coefficient of Fourier series representing Zu $u_n = \int_0^1 [Zu](\theta)\, e^{-2\pi\, i\, n\, \theta}\, d\theta$	$l^2(\mathbb{Z}) = \left\{(u_k)_{k\in\mathbb{Z}} \,:\, \sum_{k\in\mathbb{Z}} u_k^2 < \infty\right\}$
$u \in l^2_{-\epsilon}(\mathbb{Z})$	$[Zu](\theta)$ is periodic and analytic in the horizontal strip $\{-\epsilon < \text{Im } z < \epsilon\}$	$[Zu](z)$ is analytic in the annulus $\{e^{-\epsilon} < \lvert z\rvert < e^{\epsilon}\}$
	$l^2_{-\epsilon}(\mathbb{Z}) = \left\{(u_k)_{k\in\mathbb{Z}} \,:\, \sum_{k\in\mathbb{Z}} e^{2\epsilon\lvert k\rvert} u_k^2 < \infty\right\}$	u_n is the n-th coefficient of Laurent series representing Zu $u_n = \frac{1}{2\pi i} \oint_{\mathbf{C}_1} [Zu](z)\, \frac{dz}{z^{n+1}}$,

$\mathbf{C}_1$ a counter-clockwise simple closed curve parametrizing the unit circle

Z transform (cnt) and Blocking

Z-transform converts the translation operator into a multiplication operator.

$$[Z\,\tau_{\pm k}\,u]\,(z) \;=\; z^{\mp k}\,[Zu](z) \quad , \quad k \in \mathbb{Z}^{+}.$$

(order k) Constant coefficient Recurrence relation

$\downarrow$

(order k) Polynomial-typed algebraic equation.

Shift operator $\quad (\tau_k U)_J := U_{J+k}\,,\; k \in \mathbb{Z}.$

Advantage of Blocking :

- Without blocking, have r reccurence relations, one of order $2r+1$, and $r-1$ of order $r+1$
- With blocking, we have one recurrence relation of order 2

  $\Rightarrow$ one vector-valued polynomial of order 2.

Blocked recurrence relation (Example shown for order $r = 3$)

$$
\begin{array}{cccccccccccc}
 & \overset{A}{\downarrow} & & & \overset{B}{\downarrow} & & & \overset{A^t}{\downarrow} & & & & \\
\mathcal{M}_{30} & \mathcal{M}_{31} & \mathcal{M}_{32} & 2\mathcal{M}_{00} & \mathcal{M}_{01} & \mathcal{M}_{02} & \mathcal{M}_{03} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \mathcal{M}_{10} & \mathcal{M}_{11} & \mathcal{M}_{12} & \mathcal{M}_{13} & 0 & 0 & 0 & 0 & 0 \\
0 & 0 & 0 & \mathcal{M}_{20} & \mathcal{M}_{21} & \mathcal{M}_{22} & \mathcal{M}_{23} & 0 & 0 & 0 & 0 & 0 \\
\hline
0 & 0 & 0 & \mathcal{M}_{30} & \mathcal{M}_{31} & \mathcal{M}_{32} & 2\mathcal{M}_{00} & \mathcal{M}_{01} & \mathcal{M}_{02} & \mathcal{M}_{03} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \mathcal{M}_{10} & \mathcal{M}_{11} & \mathcal{M}_{12} & \mathcal{M}_{13} & 0 & 0 \\
0 & 0 & 0 & 0 & 0 & 0 & \mathcal{M}_{20} & \mathcal{M}_{21} & \mathcal{M}_{22} & \mathcal{M}_{23} & 0 & 0 \\
\hline
\end{array}
\qquad
\begin{array}{cc}
u_{J-1,0} & \\
u_{J-1,1} & \leftarrow U_{J-1} \\
u_{J-1,2} & \\
u_{J,0} & \\
u_{J,1} & \leftarrow U_J \\
u_{J,2} & \\
u_{J+1,0} & \\
u_{J+1,1} & \leftarrow U_{J+1} \\
u_{J+1,2} & \\
u_{J+2,0} & \\
u_{J+2,1} & \leftarrow U_{J+2} \\
u_{J+2,2} &
\end{array}
$$

Formal Z-transform of the Helmholtz recurrence relations

Block Z : $1 \le k \le r$, π_k projection op. onto k-th component

$$\left[\pi_k\, Z_{\mathfrak{B}}\, U\right](z) = \sum_{J=-\infty}^{\infty} u_{Jr+k}\, z^J$$

Relation with the shift operator : $k \in \mathbb{Z}^+$,

$$[Z_{\mathfrak{B}}\, \tau_{\pm k} U](z) = z^{\mp k}\,[Z_{\mathfrak{B}}\, U](z) \quad .$$

The ‘blocked’ recurrence relation at $\kappa, w = \kappa^2 h^2$

$$A(w)\, U_{J-1} + B(w)\, U_J + A^t(w)\, U_{J+1} = h\, F_J$$

after formal $Z_{\mathfrak{B}}$ becomes ,

$$[A(w)\, z + B(w) + A^t(w)\, z^{-1}] W(w,z) = h\, [Z_{\mathfrak{B}} F](z)$$

For $z \neq 0$, this is equivalent to

$$\left[A(w)\, z^2 + B(w)\, z + A^t(w)\right] W(w,z) = h\, z\, [Z_{\mathfrak{B}} F](z)$$

$$\Rightarrow \quad \mathcal{A}(w,z)\, W(w,z) \;=\; h\, z\, [Z_{\mathfrak{B}} F](z)$$

If z is such that $\det \mathcal{A}(w,z) \neq 0$, then

$$W(w,z) = \mathcal{A}^{-1}(w,z)\, h\, z\, [Z_{\mathfrak{B}} F](z).$$

Sol of the recurrence solution is given by

$$Z_{\mathfrak{B}}^{-1} W(w,z)$$

For $\kappa \notin \mathbb{R}^+$, in particular for

$$\kappa_\epsilon = \kappa\,(1 + i\epsilon)\,,\ \ \kappa \in \mathbb{R}^+\,,\ \epsilon > 0\,,$$

the above process is justified

- The problem is $l^2(\mathbb{Z})$-coercive $\rightarrow \exists\,!$ sol. in $l^2(\mathbb{Z})$.
- The unit circle $\mathcal{C}_1$ is in the region of analyticity of $W(\kappa_\epsilon^2 h, z)$
- Can take $Z_{\mathfrak{B}}^{-1}$ transform

$$\frac{1}{2\pi i} \oint_{\mathbf{C}_1} W(\kappa_\epsilon^2 h, z)\, \frac{dz}{z^{J+1}}$$

For $\kappa \in \mathbb{R}^+$, the problem is not coercive in $L^2(\mathbb{R})$ and the discretized one in $l^2(\mathbb{Z})$.

Strategy : Limiting absorbing principle.

Summary of analytic results (Part 1)

$$\mathcal{A}^{-1}(w,z) := \frac{\text{Adj } \mathcal{A}(w,z)}{\det \mathcal{A}(w,z)}.$$

Adjugate Adj $\mathcal{A}(w\,,\,z)$

$$= z^{r-2}\, Q(w,z)$$

the entries of $Q(w,z)$ are polynomial of second order in z and first order in w.

$$\mathcal{A}(w,z)$$

$$= z^2 A(w) + z\, B(w) + A^t B(w).$$

det $\mathcal{A}(w,z)$

$$= z^{r-1}\, \delta(w)\, (z^2 - 2\rho(w) z + 1)$$

$$= z^{r-1}\, \delta(w) \qquad \mathbf{q}(w,z)\,,$$

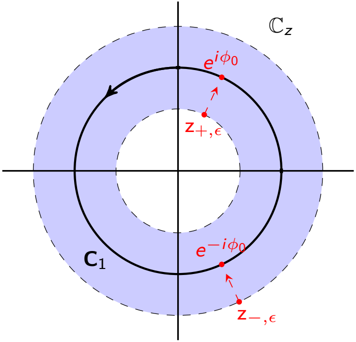
with $\rho(w)$ rational in w

$\delta(w)$ is polynomial in w.

$\kappa_\epsilon = \kappa\sqrt{1 + i\epsilon}\;,\;\; \kappa, \epsilon > 0$

Roots of $\mathbf{q}(\kappa_\epsilon^2 h^2, z)$

are denoted by $\mathrm{z}_{\pm,\epsilon}$



For w small enough, $\delta(w) \neq 0$.

$\Rightarrow$ The non-zero poles of $\mathcal{A}^{-1}(w,z)$ w.r.t z are the zeros of the characteristic poly $z \mapsto \mathbf{q}(w,z)$.

$\boxed{\text{For } \epsilon > 0 :}$ obtain solution to the recurrence relation

$$(U_\epsilon)_J = \frac{1}{2\pi i} \oint_{\mathbf{C}_1} \frac{\mathcal{A}^{-1}(\kappa_\epsilon^2 h^2, z)\, h\, z\, [Z_{\mathfrak{B}} F](z)}{z^{J+1}}\, dz$$

$\boxed{\text{For } \epsilon \to 0 :}$ by contour deformation

- ⋆ show that the limit exists, giving a solution, and
- ⋆ this resulting sol can be written as a contour integral

For $\kappa\, h\,, \epsilon > 0$ small enough,

$$|\mathrm{z}_{+,\epsilon}| < 1 < |\mathrm{z}_{-,\epsilon}|$$

$$\mathrm{z}_{\pm,\epsilon} \to e^{\pm i\phi_0}\;,\;\; \epsilon \to 0$$

Summary of analytic results (Part 2) : Dispersion Analysis

Consider $(-\Delta - \kappa^2)\,\mathbf{u} \;=\; \mathbf{f}$ with RHS $\mathbf{f}$ having Supp $F \subset [N_{\min}, N_{\max}]$, $F = (f_{J,l})$

Outgoing solution of the reccurence relation at $\kappa > 0$, $\kappa\, h < \pi$

$$u_{\text{outgoing}}(\kappa^2)_{J,0} = \frac{h \;\; e^{i\,(J\,h)\,\frac{\phi_0}{h}}}{2\,i\;\delta(\kappa^2 h^2)\;\sin\phi_0} \sum_{\substack{0 \le l \le r-1 \\ N_{\min} \le J' \le N_{\max}}} e^{i(1-\tilde{J})\phi_0}\, f_{J',l}\, \left[Q^t\left(\kappa^2 h^2, e^{-i\phi_0}\right)\right]_{(l+1)1} \;, J > N_{\max};$$

$$u_{\text{outgoing}}(\kappa^2)_{J,0} = \frac{h \;\; e^{-i\,(J\,h)\,\frac{\phi_0}{h}}}{2\,i\,\delta(\kappa^2 h^2)\;\sin\phi_0} \sum_{\substack{0 \le l \le r-1 \\ N_{\min} \le J' \le N_{\max}}} e^{i\,(J'-1)\,\phi_0}\, f_{J',l}\, \left[Q^t\left(\kappa^2 h^2, e^{i\,\phi_0}\right)\right]_{(l+1)1} \;, J < N_{\min}.$$

Analytic outgoing solution at $x = x_J = J\,h$ so that $x \notin$ Supp $\mathbf{f} = [a, b]$

$$\mathbf{u}_{\text{outgoing}}(x_J) = \frac{1}{2\,i\,\kappa}\; e^{i\;(J\;\operatorname{sgn}(J)\;h)\;\kappa}\;\hat{\mathrm{f}}(\operatorname{sgn}(J)\,\kappa).$$

The numerical wave number κ_h

is related to the argument ϕ_0

of the analytic poles of $e^{\pm i\phi_0}$ of $(\mathcal{A}(\kappa^2 h^2, z))^{-1}$.

$$\kappa_h = \frac{\phi_0}{h} = \frac{\kappa h\;(1 + \mathrm{O}(\,(\kappa\, h)^{2r})}{h}.$$

Plan

5 Pole locating algorithm and Numerical Results

Guillaume's Algorithm

At $\kappa_\epsilon = \kappa\sqrt{1+i\epsilon}$, $\epsilon, \kappa > 0$, the blocked recurrence relation after $Z_{\mathfrak{B}}$-transform gives

$$\mathcal{A}(\kappa_\epsilon^2 h^2, z)\; W(\kappa + i\epsilon, z) \;=\; h\, z\, [Z_{\mathfrak{B}} F](z).$$

Take $\epsilon \to 0$, obtain

$$\mathcal{A}(\kappa^2 h^2, z)\; W(\kappa, z) \;=\; h\, z\, [Z_{\mathfrak{B}} F](z).$$

The numerical wave number κ_h is related to the argument of the nonzero poles of $(\mathcal{A}(\kappa^2 h^2, z))^{-1}$.

Guillaume's algorithm: to look for these poles, we approximate those of $x(z)$, which solves

$$\mathcal{A}(\kappa^2 h^2, z)\, x(z) \;=\; h\, z\, b$$

for arbitrary scalar vector $b \in \mathbb{C}^r$.

Step 1: Expand b and x about an **analytic point** z_0

$$z\, h\, b = h\, z_0\, b + h\,(z - z_0)\, b$$

$$x(z) = \sum_{k=0}^{\infty} x_k(z_0)\,(z - z_0)^k.$$

Step 2 : Expand $\mathcal{A}(z)$ about z_0

$$\mathcal{A}(z) \;=\; M_0 + M_1(z - z_0) + M_2(z - z_0)^2,$$

$$M_0(z_0) = z_0 B + A^t + z_0^2 A \quad ;$$
$$M_1(z_0) = 2z_0 A + B \quad ; \quad M_2(z_0) = A\,.$$

Step 3 : The coeff. x_k solves

$$M_0(z_0)\, x_0 = h\, z_0\, b \quad ;$$
$$M_0(z_0)\, x_1 = -M_1(z_0)\, x_0 + h\, b \quad ;$$
$$M_0(z_0)\, x_k = -M_1(z_0)\, x_{k-1} - M_2(z_0)\, x_{k-2}$$
$$k \geq 2 \quad .$$

If λ_0 is the **unique closest pole** to z_0,

$$\frac{\pi_l\, x_k}{\pi_l\, x_{k+1}} \longrightarrow \lambda_0 - z_0 \ , \quad k \to \infty.$$

with π_l the projection on the l-th component of a vector.

Reference : (Thm 2.4) P. Guillaume, Nonlinear eigenproblems, Siam J. Matrix Anal. Appl. 20 (3)

Pole locating algorithm

Since the poles we look for are close to the unit circle, we consider the region $\Omega = [-2,2]\times[-2,2] \subset \mathbb{C}$, and partition it into smaller squares of width $\delta_z > 0$,

$$\Omega_{k,l} = [-2 + k\,\delta_z\,,\ -2 + (k+1)\,\delta_z] \times [-2 + l\,\delta_z\,,\ -2 + (l+1)\,\delta_z]\,.$$

The operations carried out for each square $\Omega_{i,j}$.

1. **Start** : Choose initial data $z_0 \neq 0$ arbitrarily in $\Omega_{i,j}$
   - If cond $M_0(z_0) > \epsilon_{\text{cond}}$, then z_0 is an analytic point, and continue to step 2;
   - If not, z_0 is a pole numerically, and move onto the next square.
2. Choose x_0 arbitrarily. Calculate $x_1(z_0), \ldots, x_{n_{\text{der}}+1}(z_0)$, using

$$\begin{aligned} M_0(z_0)\,x_1 &= -M_1(z_0)\,x_0 + z_0^{-1} M_0(z_0)\,x_0 \\ M_0(z_0)\,x_k &= -M_1(z_0)\,x_{k-1} - M_2(z_0)\,x_{k-2}\,,\ k \geq 2. \end{aligned}$$

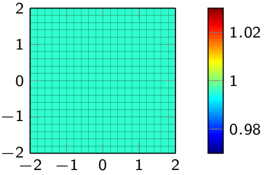
   The ratio $r = \frac{\pi_1\, x_{n_{\text{der}}+1}}{\pi_1\, x_{n_{\text{der}}}}$ gives an approximation of $\lambda_0 - z_0$, where λ_0 is the closest pole to initial data $z_0 \Rightarrow r$ gives an approximation of the direction to get from z_0 to λ_0.
3. **Restart** : Update the initial data $z_0 \longmapsto z_0 + r$.
4. **Stop criteria** :

   the condition number of M_0 , *the number of iterations N_{iter}*

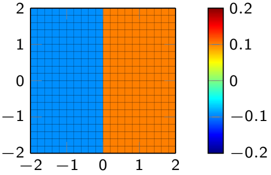
Application of Guillaume's Algorithm for Order 4

Notations :
$\mathbf{z}_{ij}$: the numerical poles calculated with Guillaume's algorithm, using initial guess from square Ω_{ij}

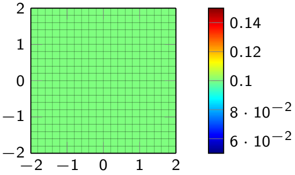
$\kappa_{h,ij}$ is obtained from $\mathbf{z}_{ij}$ by $\mathbf{z}_{ij} = e^{i\kappa_{h,ij}\, h}$



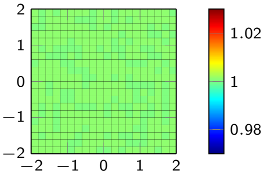
(a) Re $\mathbf{z}_{ij}$



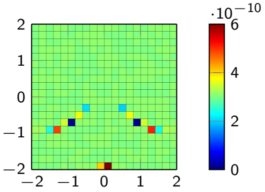
(b) Im $\mathbf{z}_{ij}$



(c) $|\text{Im } \mathbf{z}_{ij}|$



(d) Re $\kappa_{h,ij}$



(e) Im $\kappa_{h,ij}$

Parameters

Analytic wavenumber $\kappa = 1$

Discretization of $\mathbb{R}$: $h = 0.1$

Size of square Ω_{ij} : $\delta_z = 0.2$

Stop criteria

$N_{\text{iter}} = 5$; $\epsilon_{\text{cond}} = 1.e - 13$

Nb of derivatives for approx

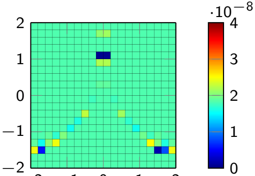
$n_{\text{der}} = 20$

Application of Guillaume's Algorithm for Order 9

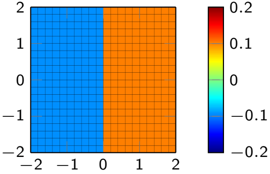
Notations :
$\mathbf{z}_{ij}$: the numerical poles calculated with Guillaume's algorithm, using initial guess from square Ω_{ij}

$\kappa_{h,ij}$ is obtained from $\mathbf{z}_{ij}$ by $\mathbf{z}_{ij} = e^{i\kappa_{h,ij}\, h}$

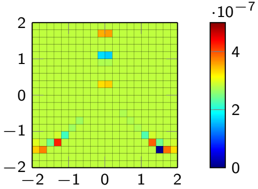
$$\mathbf{a} := \min_{1\le i,j\le 21} \text{Re } \mathbf{z}_{ij} \quad ; \quad \mathbf{b} = \min_{1\le i,j\le 21} |\text{Im } \mathbf{z}_{ij}|.$$



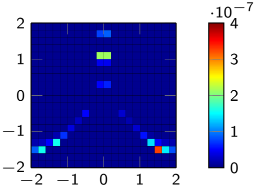
(f) $\frac{\text{Re } \mathbf{z}_{ij} - \mathbf{a}}{\mathbf{a}}$



(g) Im $\mathbf{z}_{ij}$



(h) $\frac{|\text{Img } \mathbf{z}_{ij}| - \mathbf{b}}{\mathbf{b}}$



$|\kappa_{h,ij} - 1|$

Parameters

Analytic wavenumber $\kappa = 1$

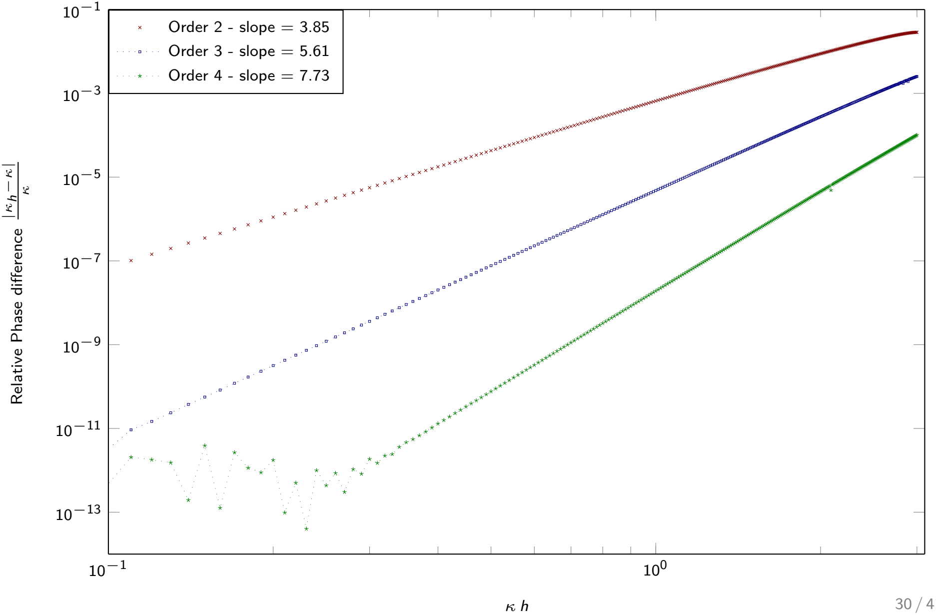
Discretization of $\mathbb{R}$: $h = 0.1$

Size of square Ω_{ij} partitioning $[-2, 2] \times [-2, 2]$: $\delta_z = 0.2$

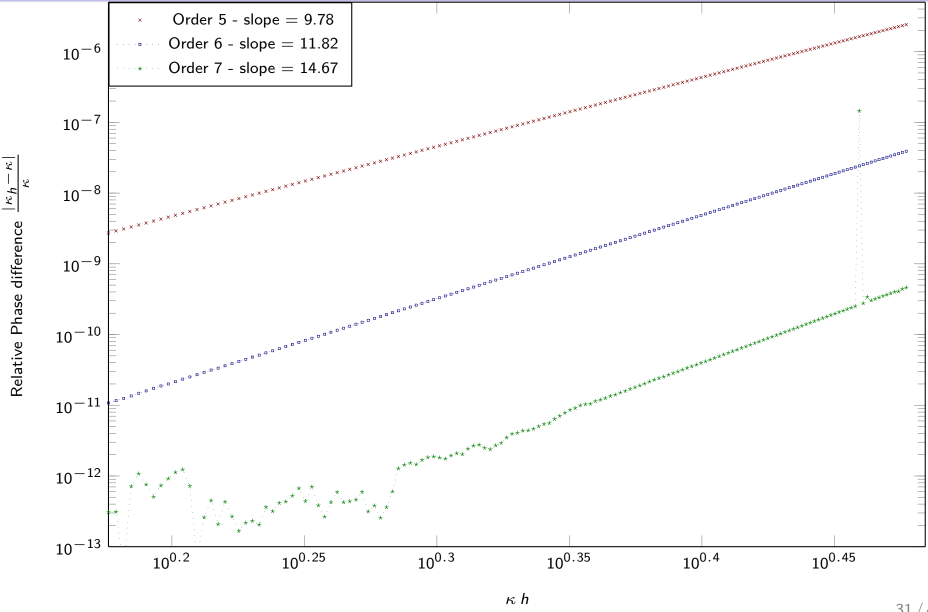
Stop criteria : $N_{\text{iter}} = 5$; $\epsilon_{\text{cond}} = 1.e - 13$

Nb of derivatives for approx $n_{\text{der}} = 20$

Numerical Dispersion Result



Numerical Dispersion Result



Plan

6. More details of analytic results

Invertibility of the local matrices

The interior matrices $\widehat{S}_{\text{int}}$, $\widehat{M}_{\text{int}}$ are symmetric and definite positive, and thus invertible.

Consider $g \in P_r(0,1)$ (polynomial of degree $\leq r$) with $g(0) = g(1) = 0$.

Define $v \in \mathbb{R}^{r-1}$ by

$$v_i := g(\tfrac{i}{r}) \; ; \; v = (v_i)_{1 \leq i \leq r-1}$$

$$\Rightarrow g(\hat{x}) := \sum_{i=1}^{r-1} v_i \hat{\phi}_i(\hat{x}).$$

We have

$$v \cdot \widehat{S}_{\text{int}}\, v = a_S\,(g, g) = \int_0^1 (g'(\hat{x}))^2\, d\hat{x} \;\; \geq 0\,;$$

$$v \cdot \widehat{M}_{\text{int}}\, v = a_M\,(g\,, g) = \int_0^1 g^2(\hat{x})\, d\hat{x} \;\; \geq 0.$$

If $v \cdot \widehat{S}_{\text{int}} v$ or $v \cdot \widehat{M}_{\text{int}} v$, then $g = 0$ i.e $v = 0$.

For $|w| < \pi^2$, $\mathcal{M}_{\text{int}}(w)$ is invertible. In addition, its inverse is analytic in w with expansion

$$\mathcal{M}_{\text{int}}^{-1}(w) = \widehat{S}_{\text{int}}^{-1} + \sum_{k=1}^{\infty} w^k \left(\widehat{S}_{\text{int}}^{-1} \widehat{M}_{\text{int}}\right)^k \widehat{S}_{\text{int}}^{-1}$$

Invertibility :

$$v \cdot \mathcal{M}_{\text{int}} v = \int_0^1 g'^2\, d\hat{x} - w \int_0^1 g^2\, d\hat{x}$$
$$\underset{\text{Poincaré inequality for } f \in H_0^1(0,1)}{\geq} (\pi^2 - w)\|g\|_{L^2}^2.$$

Since $\mathcal{M}_{\text{int}}(w) = \widehat{S}_{\text{int}} - w\widehat{M}_{\text{int}}$ is symmetric, $\mathcal{M}_{\text{int}}$ is definite positive for $w < \pi^2$

$\Rightarrow$ is invertible for such w.

Analyticity : Can show that

Spectral radius $\rho\left(\widehat{M}_{\text{int}}\, \widehat{S}_{\text{int}}^{-1}\right) \leq \pi^2$.

Thus for $|w| < \pi^2$, the Neumann series converges, giving an analytic inverse.

Structure of zeros of $\det \mathcal{A}(w,z) = \delta(w)\,\mathbf{q}(w,z) = \delta(w),(z^2 - 2\rho(w)z + 1)$

Goals - For small enough w : **1.** $\boxed{\rho(w) = \frac{\beta(w)+\det B(w)}{-2\delta(w)} = \cos w^{1/2} + w\mathrm{O}(w^r)}$; **2.** $\boxed{\delta(w) \neq 0}$

Part 1 : Show

$$\beta(w) + \det B(w) = -2\delta(w) - w\ \det \mathcal{M}_{\text{int}}(w)\left(1 + w\kappa \cdot \mathcal{M}_{\text{int}}^{-1}(w)\,\kappa\right).$$

$$\Rightarrow \frac{\beta(w)+\det B(w)}{\delta(w)} = -2 - w\frac{\det \mathcal{M}_{\text{int}}(w)}{\delta(w)}\left(1 + w\kappa \cdot \mathcal{M}_{\text{int}}^{-1}(w)\,\kappa\right)$$

Part 2 : Show $w\,\kappa \cdot \mathcal{M}_{\text{int}}^{-1}\kappa = -1 + \frac{2-2\cos w^{1/2}}{w^{1/2}\sin w^{1/2}} + \mathrm{O}(w^{2[r/2]+1})$

Part 3 : Show $-\frac{\delta(w)}{\det \mathcal{M}_{\text{int}}(w)} = \frac{w^{1/2}}{\sin w^{1/2}} + w^{2[\frac{r-1}{2}]+2}\,\mathrm{e}(\mathfrak{a},\mathfrak{b}).$

$$\kappa_j = \int_0^1 \hat{\phi}_j(\hat{x})\,d\hat{x}.$$
$$\kappa = (\kappa_1, \ldots, \kappa_{r-1})^t$$

$$1 \le j \le r-1$$
$$(\mathfrak{a}_0)_j = \widehat{S}_{jr} \qquad (\mathfrak{a}_1)_j = \widehat{M}_{jr}$$
$$(\mathfrak{b}_0)_j = \widehat{S}_{j0} \qquad (\mathfrak{b}_1)_j = \widehat{M}_{j0}$$
$$\mathfrak{a}(w) = \mathfrak{a}_0 - w\mathfrak{a}_1$$
$$\mathfrak{b}(w) = \mathfrak{b}_0 - w\mathfrak{b}_1$$

$$\begin{matrix} 2\mathcal{M}_{00} & \mathcal{M}_{01} & \cdots & \mathcal{M}_{0(r-1)} & \mathcal{M}_{0r} \\ \mathcal{M}_{10} & \mathcal{M}_{11} & \cdots & \mathcal{M}_{1(r-1)} & \mathcal{M}_{1r} \\ \vdots & \vdots & \ddots & \vdots & \vdots \\ \mathcal{M}_{(r-1)0} & \mathcal{M}_{(r-1)1} & \cdots & \mathcal{M}_{(r-1)(r-1)} & \mathcal{M}_{(r-1)r} \\ \mathcal{M}_{r0} & \mathcal{M}_{r1} & \cdots & \mathcal{M}_{r(r-1)} & \mathcal{M}_{rr} \end{matrix}$$

$\mathfrak{b}(w)$ $B(w)$ $\mathcal{M}_{\text{int}}(w)$ $\mathfrak{a}(w)$

$$B(w) = \begin{pmatrix} 2\mathcal{M}_{00}(w) & \mathfrak{b}^t(w) \\ \mathfrak{b}(w) & \mathcal{M}_{\text{int}}(w) \end{pmatrix}$$

$$\beta(w) := \det \begin{pmatrix} 0 & \mathfrak{a}^t(w) \\ \mathfrak{a}(w) & \mathcal{M}_{\text{int}}(w) \end{pmatrix}$$

$$\delta(w) := \det \begin{pmatrix} \mathcal{M}_{0r}(w) & \mathfrak{b}^t(w) \\ \mathfrak{a}(w) & \mathcal{M}_{\text{int}}(w) \end{pmatrix}$$

Structure of zeros of $\mathbf{q}(w,z) = z^2 - 2\rho(w)z + 1$ (cnt)

Part 2 : Notation : $[f] = (f(j/r))_{0\le j\le r}$

$$\kappa \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\kappa = \widehat{M}_{{\rm int},\star}\,[1] \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\widehat{M}_{{\rm int},\star}\,[1]$$
$$= \mathrm{a}_w\,(f,f) + \mathrm{O}(w^{2[r/2]}).$$
$$= -w^{-1} + \frac{2 - 2\cos w^{1/2}}{w^{3/2}\sin w^{1/2}} + w^{2[r/2]}\,\mathrm{e}(\kappa),$$

where f **is the unique solution to the BVP**

$$-f'' - wf = 1\ ;\ f(0) = f(1).$$

Part 3

Step 3a :

$$\delta(w) = \det \mathcal{M}_{\rm int}(w)\left[\widehat{S}_{r0} - w\widehat{M}_{r0} - \mathfrak{a}(w) \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\mathfrak{b}(w)\right]$$

Step 3b :

$$\begin{aligned}\mathfrak{a}(w) \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\mathfrak{b}(w) \;=\;& \mathfrak{a}_0 \cdot \widehat{S}_{\rm int}^{-1}\mathfrak{b}_0\\ &+ w\left(\widehat{S}_{\rm int}^{-1}\mathfrak{a}_0 \cdot \mathrm{Y} - \mathfrak{a}_1 \cdot \widehat{S}_{\rm int}^{-1}\mathfrak{b}_0\right)\\ &+ w^2\ \mathrm{X} \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\mathrm{Y}\quad .\end{aligned}$$

with $\mathrm{Y} := \widehat{M}_{\rm int}\widehat{S}_{\rm int}^{-1}\mathfrak{b}_0 - \mathfrak{b}_1$; $\mathrm{X} := \widehat{M}_{\rm int}\widehat{S}_{\rm int}^{-1}\mathfrak{a}_0 - \mathfrak{a}_1$

Step 3c :

$$\mathfrak{a}_0 \cdot \widehat{S}_{\rm int}^{-1}\mathfrak{b}_0 = \mathrm{a}_{\mathrm{S}}(\hat\phi_r, \hat\phi_0 + x - 1) = \widehat{S}_{r0} + 1.$$

$$\widehat{S}_{\rm int}^{-1}\mathfrak{a}_0 \cdot \mathrm{Y} - \mathfrak{a}_1 \cdot \widehat{S}_{\rm int}^{-1}\mathfrak{b}_0$$
$$= \mathrm{a}_{\mathrm{M}}(\hat\phi_r - x, x - 1) - \mathrm{a}_{\mathrm{M}}(\hat\phi_r, \hat\phi_0 + x - 1) = \tfrac{1}{6} - \widehat{M}_{r0}.$$

Step 3d :

$$\mathrm{X} \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\mathrm{Y}$$
$$= \widehat{M}_{{\rm int},\star}\,[-x] \cdot \mathcal{M}_{\rm int}^{-1}(w)\,\widehat{M}_{{\rm int},\star}\,[x-1]$$
$$= \mathrm{a}\left(\tilde f, -f'' - wf\right) + w^{2[\frac{r-1}{2}]}\mathrm{e}(\mathfrak{a},\mathfrak{b})$$
$$= -\frac{1}{w^2} - \frac{1}{6w} + \frac{1}{w^{3/2}\sin w^{1/2}} + w^{2[\frac{r-1}{2}]}\mathrm{e}(\mathfrak{a},\mathfrak{b})$$

where f and $\tilde f$ **are the unique solutions to**

$$-\tilde f'' - w\tilde f = -x\ ;\ \tilde f(0) = \tilde f(1) = 0$$
$$-f'' - wf = x - 1\ ;\ f(0) = f(1) = 0.$$

$$\begin{matrix} \mathcal{M}_{00} & \mathcal{M}_{01} & \dots & \mathcal{M}_{0(r-1)} & \mathcal{M}_{0r}\\ \mathcal{M}_{10} & \mathcal{M}_{11} & \dots & \mathcal{M}_{1(r-1)} & \mathcal{M}_{1r}\\ \vdots & \vdots & \ddots & \vdots & \vdots\\ \mathcal{M}_{(r-1)0} & \mathcal{M}_{(r-1)1} & \dots & \mathcal{M}_{(r-1)(r-1)} & \mathcal{M}_{(r-1)r}\\ \mathcal{M}_{r0} & \mathcal{M}_{r1} & \dots & \mathcal{M}_{r(r-1)} & \mathcal{M}_{rr} \end{matrix}$$

$\mathfrak{b}(w)$ $\mathcal{M}_{\rm int}(w)$ $\mathfrak{a}(w)$

$\widehat{S}_{{\rm int},\star} - w\widehat{M}_{{\rm int},\star}$

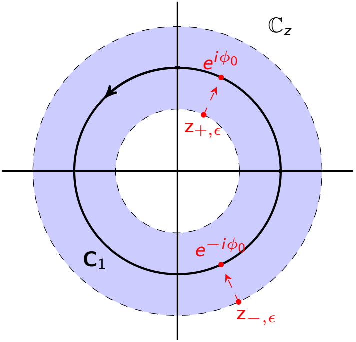
$$\mathcal{M}(w) = \widehat{S} - w\widehat{M}\ ;\ \mathcal{M}_{\rm int}(w) = \widehat{S}_{\rm int} - w\widehat{M}_{\rm int}$$
$$\mathfrak{a}(w) = \mathfrak{a}_0 - w\mathfrak{a}_1\ ;\ \mathfrak{b}(w) = \mathfrak{b}_0 - w\mathfrak{b}_1$$

Limiting absorption principle . Outgoing solution

$$\mathbf{q}(w,z) = z^2 - 2\rho(w)z + 1$$

$$\rho(w) = \cos w^{1/2} + w\mathrm{O}(w^r).$$

Discri. $\Delta(w) = -4\sin^2(w^{1/2})\,(1+\mathrm{O}(w^r))$



$$z_{\pm,\epsilon} := \rho(\kappa_\epsilon^2 h^2) \pm \tfrac{1}{2}\sqrt{\Delta(\kappa_\epsilon^2 h^2)}.$$

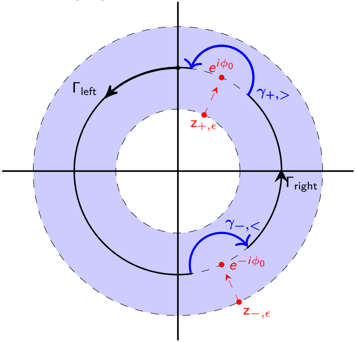
$$z_{\pm,0} = e^{\pm i\phi_0} := \rho(\kappa h) \pm \tfrac{1}{2} i \sqrt{|\Delta(\kappa^2 h^2)|}.$$

$$\cos\phi_0 = \rho(\kappa^2 h^2) = \cos(\kappa h) + (\kappa h)^2\,\mathrm{O}((\kappa h)^{2r})$$

$$\Rightarrow \quad \phi_0 \quad = \kappa h\ (1\ +\ \mathrm{O}(\,(\kappa h)^{2r}\,)\,.$$

$$(U_\epsilon)_J = \frac{1}{2\pi i}\oint_{\mathbf{C}_1} \frac{\mathcal{A}^{-1}(\kappa_\epsilon^2 h^2, z)\, h\, z\, [Z_{\mathfrak{B}} F](z)}{z^{J+1}}\, dz$$
$$= \frac{1}{2\pi i}\oint_{\Gamma_{\text{outgoing}}} \frac{\mathcal{A}^{-1}(\kappa_\epsilon^2 h^2, z)\, h\, z\, [Z_{\mathfrak{B}} F](z)}{z^{J+1}}\, dz$$

$$(U_{\text{outgoing}})_J = \lim_{\epsilon\to 0^+}(U_\epsilon)_J$$
$$= \frac{1}{2\pi i}\oint_{\Gamma_{\text{outgoing}}} \frac{\mathcal{A}^{-1}(\kappa^2 h^2, z)\, h\, z\, [Z_{\mathfrak{B}} F](z)}{z^{J+1}}\, dz$$



$\mathbf{C}_1$ is deformed to Γ_{outgoing}

$\Gamma_{\text{outgoing}} := \Gamma_{\text{right}} \cup \gamma_{+,>} \cup \Gamma_{\text{left}} \cup \gamma_{-,<}$.

Numerical wavenumber (Part 1)

Goal : obtain the explicit formula for the outgoing solution of the reccurence relation at $\kappa > 0$.

$$u_{\text{outgoing}}(\kappa^2)_{J,0} = \frac{h\, e^{i\,J\,\phi_0}}{2\,i\;\delta(\kappa^2 h^2)\,\sin\phi_0} \sum_{\substack{0\le l\le r-1\\ N_{\min}\le J'\le N_{\max}}} e^{i(1-\tilde{J})\phi_0}\, f_{J',l}\,\left[Q^t\left(\kappa^2 h^2, e^{-i\phi_0}\right)\right]_{(l+1)1}\;, J > N_{\max};$$

$$u_{\text{outgoing}}(\kappa^2)_{J,0} = \frac{h\, e^{-i\,J\,\phi_0}}{2\,i\,\delta(\kappa^2 h^2)\,\sin\phi_0} \sum_{\substack{0\le l\le r-1\\ N_{\min}\le J'\le N_{\max}}} e^{i\,(J'-1)\,\phi_0}\, f_{J',l}\,\left[Q^t\left(\kappa^2 h^2, e^{i\,\phi_0}\right)\right]_{(l+1)1}\;, J < N_{\min}.$$

After this step, by using : $\phi_0 = \kappa\, h\,(1 + \mathrm{O}(\,(\kappa h)^{2r}\,)$, obtain

Dispersion Analysis

$$\kappa \;=\; \frac{\phi_0}{h} \;=\; \kappa \;+\; \kappa\,\mathrm{O}(\,(\kappa\, h)^{2r}\,) \quad .$$

Numerical wavenumber (cnt) : Explicit expression for outgoing sol

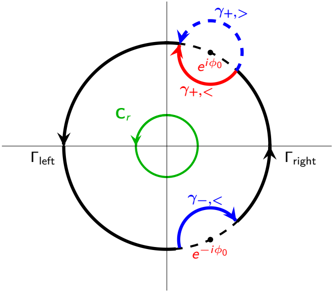
$$\mathcal{A}^{-1}(\kappa^2 h^2, z) = \frac{r^{r-2} Q(\kappa^2 h^2, z)}{z^{r-1}\, \delta(\kappa^2 h^2)\, \mathbf{q}(\kappa^2 h^2, z)} = \frac{Q(\kappa^2 h^2, z)}{z\ \delta(\kappa^2 h^2)\, (z - e^{i\phi_0})(z + e^{i\phi_0})}\ ,\ z \neq e^{\pm i\phi_0}\ .$$

$$\begin{aligned}
(U_{\text{outgoing}})_J = \lim_{\epsilon \to 0^+} (U_\epsilon)_J &= \frac{1}{2\pi i} \oint_{\Gamma_{\text{outgoing}}} \frac{\mathcal{A}^{-1}(\kappa^2 h^2, z)\, h\, z\, [Z_{\mathfrak{B}} F](z)}{z^{J+1}}\, dz \\
&= \frac{1}{2\pi i} \oint_{\Gamma_{\text{outgoing}}} \frac{Q(\kappa^2 h^2, z)}{\delta(\kappa^2 h^2)\, (z - e^{i\phi_0})(z + e^{i\phi_0})} \frac{h\, [Z_{\mathfrak{B}} F](z)}{z^{J+1}}\, dz \\
&= \frac{1}{2\pi i} \oint_{\Gamma_{\text{outgoing}}} \frac{W_0(z)}{z^{J+1}}\, dz \quad .
\end{aligned}$$

Numerical wavenumber (cnt) : Explicit expression for outgoing sol

RHS $\mathbf{f}$ having Supp $F \subset [N_{\min}, N_{\max}]$, $F = (f_{J,l})$, write the integrand as

$$z^{-J-1} W_0(z)\, dz = \frac{h\ Q(\kappa^2 h^2, z)}{\delta(\kappa^2 h^2)\ \mathbf{q}(\kappa^2 h^2, z)} z^{-J-1} \sum_{j=N_{\min}}^{N_{\max}} z^j \left(f_{j,k}\right)_{0\le k\le r-1} dz$$



Deform Γ_{outgoing} to Γ_+.

$\Gamma_+ := \Gamma_{\text{right}} \cup \gamma_{+,<} \cup \Gamma_{\text{left}} \cup \gamma_{-,<}$

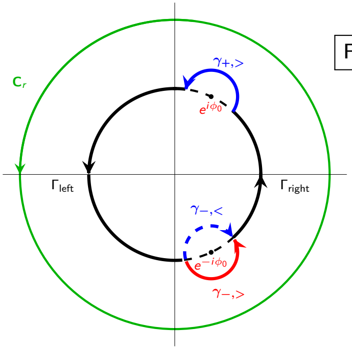
Γ_+ is homotopic to $\mathbf{C}_r$, $r < 1$.

$\boxed{\text{For } J < N_{\min} :}$ $\dfrac{W_0(z)}{z^{J+1}}$ **is analytic at** $z = 0$

$$\begin{aligned}
&(U_{\text{outgoing}})_J \\
&= \frac{1}{2\pi i}\left(\oint_{\Gamma_+} + \oint_{\gamma_{+,>}\ \cup\ -\gamma_{+,<}}\right) \frac{W_0(z)}{z^{J+1}}\, dz \\
&= \frac{1}{2\pi i}\oint_{\mathbf{C}_r} \frac{W_0(z)}{z^{J+1}}\, dz + \operatorname{Res}\left(\frac{W_0(z)}{z^{J+1}}, e^{i\phi_0}\right) ,\ r<1 \\
&= \operatorname{Res}\left(\frac{W_0(z)}{z^{J+1}}\ ,\ e^{i\phi_0}\right) \\
&= \frac{h\ Q(\kappa^2 h^2, e^{i\phi_0})\ [Z_{\mathfrak{B}} F](e^{i\phi_0})}{\delta(\kappa^2 h^2)\ \left(e^{i\phi_0} - e^{-i\phi_0}\right)} \left(e^{i\phi_0}\right)^{-J-1}.
\end{aligned}$$

Numerical wavenumber (cnt) : Explicit expression for outgoing sol

$$\text{For } \tilde{z} := z^{-1} \; : \; z^{-J} W_0(z)\, \frac{dz}{z} = \frac{h}{\delta(\kappa^2 h^2)} \frac{Q^t(\kappa^2 h^2, \tilde{z})}{\mathbf{q}(\kappa^2 h^2, \tilde{z})} \tilde{z}^J \sum_{j=N_{\text{min}}}^{N_{\text{max}}} \tilde{z}^{-j} \left(f_{j,k}\right)_{0 \le k \le r-1} \frac{d\tilde{z}}{\tilde{z}}.$$



Deform Γ_{outgoing} to Γ_- ;

$\Gamma_- := \Gamma_{\text{right}} \cup \gamma_{+,>} \cup \Gamma_{\text{left}} \cup \gamma_{-,>}$

Γ_- is homotopic to $\mathbf{C}_r$, $r > 1$.

$\boxed{\text{For } J > N_{\text{max}} :}$ $N_{\text{min}} \le j \le N_{\text{max}} \Rightarrow J - j - 1 \ge J - N_{\text{max}} - 1 \ge 0$

$\Rightarrow$ the integrand is analytic at $\tilde{z} = 0$.

$$(U_{\text{outgoing}})_J = \frac{1}{2\pi i} \left(\oint_{\Gamma_{\text{outgoing}}} + \oint_{\gamma_{-,<} \cup -\gamma_{-,>}} \right) \frac{W_0(z)}{z^{J+1}} dz$$

$$= \frac{1}{2\pi i} \oint_{\mathbf{C}_r} \frac{W_0(z)}{z^{J+1}} dz - \text{Res}\left(\frac{W_0(z)}{z^{J+1}}, e^{-i\phi_0} \right) \quad , \quad 1 < r$$

$$= \frac{1}{2\pi i} \oint_{\mathbf{C}_{r^{-1}}} \frac{h\, \tilde{z}^J}{\delta(\kappa^2 h^2)} \frac{Q^t(\kappa^2 h^2, \tilde{z})}{\mathbf{q}(\kappa^2 h^2, \tilde{z})} [Z_{\mathfrak{B}} F](\tilde{z}^{-1}) \frac{d\tilde{z}}{\tilde{z}}$$

$$- \text{Res}\left(\frac{W_0(z)}{z^{J+1}}, e^{-i\phi_0} \right) \quad , \quad 1 < r$$

$$= -\text{Res}\left(W_0(z)\, z^{-(J+1)}, e^{-i\phi_0} \right)$$

$$= -\frac{h}{\delta(\kappa^2 h^2)} \frac{Q(\kappa^2 h^2, e^{-i\phi_0})\, [Z_{\mathfrak{B}} F](e^{-i\phi_0})}{(e^{-i\phi_0} - e^{i\phi_0})} (e^{-i\phi_0})^{-J-1}.$$

Conclusion

Thank you for your attention